Appendix D

Complete Calpuff

Class I Increment Results

for MRY SO_2

Calpuff Class I Increment Results
TRNP - North Unit
($\mu g/m^3$)

	1990	1991	1992	1993	1994
3-hr Predictions					
Highest	36.2	77.7	36.9	43.5	35.8
High, 2nd High	26.7	43.0	32.4	30.5	26.4
Max # of Exceedances*	2	9	7	3	2
Max # sig. MRY contrib. to violations*	1	8	3	1	0
24-hr Predictions					
Highest	15.2	18.3	11.5	15.2	11.4
High, 2nd High	10.5	12.7	8.2	10.9	9.8
Max # of Exceedances*	12	14	19	20	22
Max # sig. MRY contrib. to violations*	9	11	10	12	10
Max Annual Prediction	1.38	1.36	1.36	1.42	1.53

*   Worst-case receptor

Calpuff Class I Increment Results
TRNP - Elkhorn Ranch Unit
($\mu g/m^3$)

	1990	1991	1992	1993	1994
3-hr Predictions					
Highest	40.4	22.4	21.2	22.6	34.5
High, 2nd High	36.5	21.5	20.7	20.6	26.2
Max # of Exceedances*	2	0	0	0	2
Max # sig. MRY contrib. to violations*	0	0	0	0	0
24-hr Predictions					
Highest	11.4	13.5	8.9	9.0	13.6
High, 2nd High	10.2	10.4	6.3	7.4	13.2
Max # of Exceedances*	7	10	5	8	10
Max # sig. MRY contrib. to violations*	4	5	4	6	6
Max Annual Prediction	0.84	0.95	0.86	0.85	0.98

*   Worst-case receptor

Calpuff Class I Increment Results
Lostwood Wilderness Area
($\mu g/m^3$)

	1990	1991	1992	1993	1994
3-hr Predictions					
Highest	22.5	23.4	38.5	37.4	28.8
High, 2nd High	20.4	22.1	34.3	23.1	19.1
Max # of Exceedances*	0	0	5	1	1
Max # sig. MRY contrib. to violations*	0	0	4	0	0
24-hr Predictions					
Highest	8.0	9.1	8.5	8.3	8.1
High, 2nd High	7.7	7.3	6.9	6.9	7.8
Max # of Exceedances*	7	15	9	5	10
Max # sig. MRY contrib. to violations*	5	14	8	3	8
Max Annual Prediction	0.49	0.74	0.69	0.49	0.57

*   Worst-case receptor

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Calpuff Class I Increment Results
Medicine Lake Wilderness Area
(μg/m^3)

	1990	1991	1992	1993	1994
3-hr Predictions					
Highest	39.4	12.3	17.7	19.4	16.3
High, 2nd High	30.2	11.1	16.6	18.9	15.9
Max # of Exceedances*	2	0	0	0	0
Max # sig. MRY contrib. to violations*	1	0	0	0	0
24-hr Predictions					
Highest	10.6	3.4	7.9	7.4	7.0
High, 2nd High	5.4	3.2	5.6	7.1	5.5
Max # of Exceedances*	2	0	3	3	4
Max # sig. MRY contrib. to violations*	1	0	2	2	3
Max Annual Prediction	0.25	0.17	0.26	0.21	0.25

*   Worst-case receptor

Calpuff Class I Increment Results
Fort Peck Reservation
($\mu g/m^3$)

	1990	1991	1992	1993	1994
3-hr Predictions					
Highest	34.3	16.5	25.5	22.1	20.1
High, 2nd High	33.5	14.6	22.2	18.8	17.8
Max # of Exceedances*	2	0	1	0	0
Max # sig. MRY contrib. to violations*	1	0	0	0	0
24-hr Predictions					
Highest	10.5	5.8	9.7	8.1	8.2
High, 2nd High	5.8	4.9	5.4	6.7	7.4
Max # of Exceedances*	2	1	3	3	4
Max # sig. MRY contrib. to violations*	1	0	2	2	3
Max Annual Prediction	0.24	0.18	0.27	0.20	0.28

*   Worst-case receptor

Appendix E

National Park Service

Transmittal

NATIONAL PARK SERVICE
AIR RESOURCES DIVISION

P.O. BOX 25287, Denver, CO 80225-0287

FACSIMILE COVER SHEET

Date: 3/10/99

Telephone: 303-969-2079
Fax: (303) 969-2822

To: STEVE WEBER

From: John NOTAR

Subject: REGIONAL HAZE CALCULATIONS

Steve: GIVE ME A CALL IF YOU HAVE ANY QUESTIONS

John

Number of Pages:
(Including this cover sheet) 9

Office Location: 7333 W. Jefferson, Room 450, Lakewood, CO 80235

(Send Mail to: 12795 W. Alameda Parkway, Lakewood, CO 80228)

DRAFT 2/8/99

Class I Area Name	Land Management Type	IMPROVE Aerosol Site Code	IMPROVE RH Site Code	Aerosol Analysis Region	RH Analysis Region	Values Based on the Mean o Non Hygroscopic Extinction			
						Autumn	Spring	Summer	Winter
Lostwood	Wilderness			WRA	WUS	5.36	5.30	8.85	4.02
Medicine Lake	Wilderness			WRA	WUS	5.36	5.30	8.85	4.02
Theodore Roosevelt	National Park			WRA	WUS	5.36	5.30	8.85	4.02

BACKGROUND EXTINCTION   NOTE: NOMINAL RAYLEIGH = 10.0

FALL $5.36 + (1.44)(1.85) + 10 = 18.02$ Mm^{-1}

SPRING $5.3 + (1.65)(2.01) + 10 = 18.62$ Mm^{-1}

SUMMER $8.85 + (2.72)(1.65) + 10 = 23.34$ Mm^{-1}

WINTER $4.02 + (1.44)(2.44) + 10 = 17.53$ Mm^{-1}
           1.03
           16.53

f the Cleanest 20% of Days
   Dry Hygroscopic Extinction

Values Based on Mean of all Sample Days w/16 or more valid hours
Average f(RH)

Autumn	Spring	Summer	Winter	Annual	Autumn	Spring	Summer	Winter
1.44	1.65	2.72	1.03	1.99	1.85	2.01	1.65	2.44
1.44	1.65	2.72	1.03	1.99	1.85	2.01	1.65	2.44
1.44	1.65	2.72	1.03	1.99	1.85	2.01	1.65	2.44
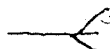
Appendix 2.B

Visibility Parameters

Visibility is usually characterized by either visual range (VR) (the greatest distance that a large dark object can be seen) or by the light-extinction coefficient (b_{ext}) (the attenuation of light per unit distance due to scattering and absorption by gases and particles in the atmosphere) (IMPROVE, 1996). Under certain assumed conditions, these parameters are inversely related to each other by Equation 1. The dimensions of VR are length and the dimensions of b_{ext} are 1/length. Visual range is usually expressed in kilometers. The extinction coefficient is sometimes expressed as "inverse kilometers" (km^{-1}) or as "inverse megameters" (Mm^{-1}) (the reciprocal of 1 million meters). If b_{ext} is expressed in Mm^{-1} the coefficient 3.912 becomes 3912 as in Equation 1.

$$VR(km) = \frac{3.912}{b_{ext}(km^{-1})} = \frac{3912}{b_{ext}(Mm^{-1})}$$

Equation 1. Relationship between visual range and light-extinction coefficient.

Other visibility parameters frequently used include)E and contrast. These metrics relate to the color difference or contrast, respectively, of a plume or haze with respect to some viewing background.

Calculating the Extinction Coefficient

Visibility is degraded by visible light scattered into and out of the line of sight and by light absorbed along the line of sight. Light extinction is the sum of light scattering and absorption, and is usually quantified using the light extinction coefficient (b_{ext}). Using a generalized approach to estimating visibility effects, one can calculate the extinction coefficient as the sum of its parts, i.e., $b_{ext} = b_{scat} + b_{abs}$, where b_{scat} and b_{abs} are the light scattering and absorption coefficients. The light scattering and absorption coefficients can be further broken down by their respective components. The scattering coefficient is affected by light scattering (Rayleigh scattering (b_{Ray})) from air molecules and from particle scattering (b_{sp}); the particles can be natural aerosol or result from air pollutants. The absorption coefficient is affected by gaseous absorption (b_{ag}) and particulate absorption (b_{ap}). Nitrogen dioxide is the only major light-absorbing gas in the lower atmosphere; it generally does not affect hazes, although it can be an important element in a coherent plume assessment. Therefore, only particle absorption is considered in the suggested visibility analyses.

Particle scattering can be broken down by the contributions of different particulate species. It has been convenient to consider the scattering coefficients of fine particles ($PM_{2.5}$) (particles with mass mean diameters less than or equal to 2.5 µm) and coarse particles (mass mean diameters

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greater than 2.5μm but less than or equal to 10μm). The fine particle scattering coefficient can be further defined by the sum of the scattering coefficient due to sulfates (b_{SO4}), nitrates (b_{NO3}), organic aerosols (b_{OC}), and soil (b_{Soil}); the coarse scattering coefficient (b_{Coarse}) is not refined any further. Thus the particle scattering coefficient (b_{sp}) can be expressed as in Equation 2.

$$b_{sp} = b_{SO4} + b_{NO3} + b_{OC} + b_{Soil} + b_{Coarse}$$

Equation 2. Components of particle scattering.

Each of the particle scattering coefficients can be related to the mass of the components using the relationships in Equation 3.

$$
\begin{aligned}
b_{SO4} &= 3\left[(NH_4)_2SO_4\right]f(RH) \\
b_{NO3} &= 3\left[NH_4NO_3\right]f(RH) \\
b_{OC} &= 4\left[OC\right] \\
b_{Soil} &= 1\left[Soil\right] \\
b_{Coarse} &= 0.6\left[Coarse\ Mass\right]
\end{aligned}
$$

Equation 3. Relationship between particle scattering and mass of each species.

The quantities in brackets are the masses expressed in μg/m³. (It is assumed that the forms of the $SO_4^=$ and NO_3^- are ammonium sulfate [$(NH_4)_2SO_4$] and ammonium nitrate [NH_4NO_3].) The numeric coefficients are the "dry" scattering efficiencies (m²/g). The term f(RH) is the relative humidity adjustment factor. The extinction coefficients are in Mm⁻¹. If the "dry" scattering efficiencies are divided by 1000 (i.e., 0.003 instead of 3) the resultant extinction coefficients will be in km⁻¹.

Particle absorption (b_{ap}) is primarily due to elemental carbon (soot). For purposes of analyzing the effects of soot on visibility in a modeling analysis, the relationship in Equation 4 should be used. Again, the quantity in brackets is the mass of elemental carbon in μg/m³ and 10 is the extinction efficiency.

$$b_{ap} = 10\left[EC\right]$$

Equation 4. Relationship between particle absorption and elemental carbon.

The total atmospheric extinction can be expressed as in Equation 5.

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$$b_{ext} = b_{SO4} + b_{NO3} + b_{OC} + b_{soil} + b_{Coarse} + b_{ap} + b_{Ray}$$

Equation 5 – Components of Extinction

To the extent that a source contributes to the formation of some of these constituents, those contributions can be summed to yield the source's contribution to extinction. This will be discussed in more detail below.

Examination of Equation 3 reveals that the sulfate and nitrate components of the extinction coefficient are dependent upon relative humidity. These aerosols are hygroscopic and the addition of water enhances their scattering efficiencies. It is sometimes convenient to consider the sulfate and nitrate components of extinction separately from the remaining components of Equation 5 and to keep the relative humidity adjustment factor (f(RH)) separate. Equation 5 can then be rewritten as in Equation 6, where b_{SN} is the combined extinction coefficient of sulfate and nitrate, excluding the relative humidity adjustment factor, and b_{dry} is the sum of b_{OC}, b_{Soil}, b_{Coarse}, b_{ap}, and b_{Ray}.

$$b_{ext} = b_{SN} f(RH) + b_{dry}$$

Equation 6– Extinction coefficient expressed as the sulfate and nitrate contribution ($b_{SN} = 3[(NH_4)_2SO_4 + NH_4NO_3]$) and non-hygroscopic components ($b_{dry} = b_{OC}+b_{Soil}+b_{Coarse}+b_{ap}+b_{Ray}$).

The relative humidity adjustment factor requires some further explanation. The variation of the effect of relative humidity on the extinction efficiency, f(RH), of sulfates and nitrates is given numerically in Table B-1. As can be seen, the effect of relative humidity on the extinction efficiency of these aerosols is non-linear, and is several times greater at higher relative humidity than at lower humidity.

FLAG proposes that the relative humidity correction to the "dry" scattering efficiencies (unadjusted for relative humidity) for hygroscopic particles are made as follows:

- FLAG recommends using historic averages of *f(RH)* for the Class I area(s) of concern.

- If it is desired to apply day-by-day *f(RH)* corrections to the analysis, then hourly, concurrent (with the collection of the 24-hour particle measurements) relative humidity data are required. The corresponding hourly f(RH) values should be averaged to generate a 24-hour relevant *f(RH)* factor. FLAG recommends, however, that if the hourly relative humidity exceeds 98%, that it be rolled back to 98%, so that there will be no *f(RH)* factors applied that are greater than f (98%).

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These factors are applicable on a short-term basis. If the particulate concentrations are only available over a longer averaging time (*e.g.*, a 24-hour sample or a seasonal average) then the average relative humidity adjustment factor for that time period must be applied not a factor based the average relative humidity. (Alternately, short-term extinction coefficients (i.e., 1-hour) may be averaged to yield a longer-term average.)

Table 2.B-1. f(RH) values for various values of relative humidity

RH(%)	F(RH)	RH(%)	F(RH)	RH(%)	F(RH)	RH(%)	F(RH)
1	1.0000	26	1.0122	51	1.2368	76	2.2630
2	1.0000	27	1.0126	52	1.2512	77	2.3565
3	1.0000	28	1.0130	53	1.2671	78	2.4692
4	1.0000	29	1.0135	54	1.2844	79	2.6011
5	1.0000	30	1.0139	55	1.3018	80	2.7330
6	1.0000	31	1.0173	56	1.3234	81	2.8461
7	1.0000	32	1.0206	57	1.3450	82	2.9592
8	1.0000	33	1.0254	58	1.3695	83	3.0853
9	1.0000	34	1.0315	59	1.3969	84	3.2245
10	1.0000	35	1.0377	60	1.4243	85	3.3637
11	1.0000	36	1.0486	61	1.4628	86	3.5743
12	1.0000	37	1.0596	62	1.5014	87	3.7849
13	1.0000	38	1.0751	63	1.5468	88	4.0466
14	1.0001	39	1.0951	64	1.5992	89	4.3594
15	1.0001	40	1.1151	65	1.6516	90	4.6721
16	1.0004	41	1.1247	66	1.6991	91	5.3067
17	1.0006	42	1.1343	67	1.7466	92	5.9412
18	1.0024	43	1.1436	68	1.7985	93	6.9627
19	1.0056	44	1.1525	69	1.8549	94	8.3710
20	1.0089	45	1.1615	70	1.9113	95	9.7793
21	1.0097	46	1.1724	71	1.9596	96	12.4288
22	1.0105	47	1.1833	72	2.0080	97	15.0773
23	1.0111	48	1.1955	73	2.0596	98	18.0590
24	1.0115	49	1.2090	74	2.1146	99	21.3709
25	1.0118	50	1.2224	75	2.1695	100	-

Example Problem

IV.   Example Problem

It is expected that all applicants and FLMs have experience with the near field modeling application so no specific example needs to be supplied here. The distant/multi-source application does involve some new concepts, so an example application is being provided.

For the purposes of this example, let us assume that a dispersion model has been run and yielded concentrations of $SO_4^=$ (sulfate) and soot (elemental carbon). From these concentrations the analyst can calculate a change in extinction using the procedures given in Appendix B.

First, we will consider the current visibility condition (for an actual case, the applicant can turn to Appendix C). If the current 24-hour average visibility (mean of the 20% clearest days for the clearest season) at the Class I area of interest has a hygroscopic component (combined sulfate and nitrate extinction coefficient (b_{SN})) of 1.8 Mm^{-1} (neglecting the effects of relative humidity) and a nonhygroscopic component (extinction coefficient from the other components (b_{dry}) plus Rayleigh) of 19.6 Mm^{-1}, then the current extinction (b_{back}), expressed in the form of Equation 6 (Appendix B) would be:

$$b_{back} = 1.8\, f(RH) + 19.6$$

In a typical modeling analysis, IWAQM recommends and the FLMs endorse the use of five years of meteorological data. This will produce a corresponding number of 24-hour averaging periods, which will each need to be compared with the current condition. For this example we will assume that the sources in the analysis contributed 0.218 $\mu g/m^3$ of sulfate (SO_4^-) and 0.10 $\mu g/m^3$ of soot (elemental carbon). The first step is to convert the mass of $SO_4^=$ to ammonium sulfate ($(NH_4)_2SO_4$), which is accomplished by multiplying by the ratio of the molecular weights of $(NH_4)_2SO_4$ to $SO_4^=$, which is 1.375. This yields a concentration of $(NH_4)_2SO_4$ of 0.3 $\mu g/m^3$. This is then multiplied by the "dry" scattering efficiency of $(NH_4)_2SO_4$ (which is 3, from Appendix B, Equation 3), yielding an extinction coefficient for the sulfate of 0.9 Mm^{-1}; the relative humidity adjustment has not yet been applied.

In this example our modeling does not require any conversion of the mass of soot, so we will just multiply the soot concentration (0.10 $\mu g/m^3$) by the extinction efficiency of elemental carbon (which is 10, from Appendix B, Equation 4). This yields an extinction coefficient of 1.0 Mm^{-1}. Therefore, following the form of Equation 6 (Appendix B), the source contribution would be:

$$b_{source} = 0.9\, f(RH) + 1.0$$

The representative, hourly RH values for this day need to be obtained. For each hour, the corresponding f(RH) must be obtained from a table, such as that in Appendix B. These values are then averaged together. Let us assume that for this day the average f(RH) is 3.4. With the average relative humidity adjustment factor (f(RH)) of 3.4, b_{back} would be 25.72 Mm^{-1} (corresponding to a visual range of 152 km from Appendix B, Equation 1) and b_{source} would be 4.06 Mm^{-1}, the resulting change in extinction being 16%. These calculations would have to be repeated for each 24-hour average concentration in the analysis, using the corresponding average f(RH). To portray the frequency, magnitude, and geographic extent of expected impairment, this calculation will have to be repeated for all days and many receptors in the modeling domain. FLAG expects a robust selection of model receptor locations in the Class I area be included in the analyses, *i.e.*, one receptor representing the entire area, or just the nearest boundary, will generally not be sufficient.

These factors are applicable on a short-term basis. If the particulate concentrations are only available over a longer averaging time (*e.g.*, a 24-hour sample or a seasonal average) then the average relative humidity adjustment factor for that time period must be applied <u>not</u> a factor based the average relative humidity. (Alternately, short-term extinction coefficients (i.e., 1-hour) may be averaged to yield a longer-term average.)

Table 2.B-1. f(RH) values for various values of relative humidity

RH(%)	F(RH)	RH(%)	F(RH)	RH(%)	F(RH)	RH(%)	F(RH)
1	1.0000	26	1.0122	51	1.2368	76	2.2630
2	1.0000	27	1.0126	52	1.2512	77	2.3565
3	1.0000	28	1.0130	53	1.2671	78	2.4692
4	1.0000	29	1.0135	54	1.2844	79	2.6011
5	1.0000	30	1.0139	55	1.3018	80	2.7330
6	1.0000	31	1.0173	56	1.3234	81	2.8461
7	1.0000	32	1.0206	57	1.3450	82	2.9592
8	1.0000	33	1.0254	58	1.3695	83	3.0853
9	1.0000	34	1.0315	59	1.3969	84	3.2245
10	1.0000	35	1.0377	60	1.4243	85	3.3637
11	1.0000	36	1.0486	61	1.4628	86	3.5743
12	1.0000	37	1.0596	62	1.5014	87	3.7849
13	1.0000	38	1.0751	63	1.5468	88	4.0466
14	1.0001	39	1.0951	64	1.5992	89	4.3594
15	1.0001	40	1.1151	65	1.6516	90	4.6721
16	1.0004	41	1.1247	66	1.6991	91	5.3067
17	1.0006	42	1.1343	67	1.7466	92	5.9412
18	1.0024	43	1.1436	68	1.7985	93	6.9627
19	1.0056	44	1.1525	69	1.8549	94	8.3710
20	1.0089	45	1.1615	70	1.9113	95	9.7793
21	1.0097	46	1.1724	71	1.9596	96	12.4288
22	1.0105	47	1.1833	72	2.0080	97	15.0773
23	1.0111	48	1.1955	73	2.0596	98	18.0590
24	1.0115	49	1.2090	74	2.1146	99	21.3709
25	1.0118	50	1.2224	75	2.1695	100	-

Appendix F

Calpost Code Changes

The following section of Calpost (Version 5.0, Level 981116) function GROWTH
was changed from:

```
      if(mvisbk.EQ.1) then

c ---      Original IWAQM(1993) curve
           if(rh.le.0.3)then
              growth = 1.0
           elseif(rh.le.0.8) then
              growth = 0.7/(1.-rh)
           elseif(rh.lt.rhmax)then
              growth = 0.8064/(1.0304-rh)
           else
              growth = 0.8064/(1.0304-rhmax)
           endif

      elseif(mvisbk.EQ.2) then

c ---      IMPROVE report, July 1996, tabulation
```

to:

```
c      if(mvisbk.EQ.1) then

c ---      Original IWAQM(1993) curve
c          if(rh.le.0.3)then
c             growth = 1.0
c          elseif(rh.le.0.8) then
c             growth = 0.7/(1.-rh)
c          elseif(rh.lt.rhmax)then
c             growth = 0.8064/(1.0304-rh)
c          else
c             growth = 0.8064/(1.0304-rhmax)
c          endif

      if(mvisbk.EQ.1 .OR. mvisbk.EQ.2) then

c ---      IMPROVE report, July 1996, tabulation
```

Appendix G

Description of Files

on

Accompanying Computer Media

NDDH computer files related to the Calpuff Class I analysis for MRY
station are provided on computer media accompanying this report.
An attempt was made to include all files which might be of interest
to the reviewer.

The computer media includes three primary directories (INPUT,
OUTPUT, PROG) and a number of sub-directories. Directory structure
and naming scheme should be fairly intuitive. Each sub-directory
includes an index file (INDEX.TXT) which describes each of the
files contained in the sub-directory.

Calpuff was executed on the basis of individual years of
meteorological data. A single set of Calpuff input control files
are provided in sub-directory PUFF of directory INPUT, i.e., input
files are not provided for each year of meteorological data (1990-
1994). Output files (sub-directories PUFF, POST, XCEED of
directory OUTPUT) are included for each year of meteorological
data. A single sub-directory index file is provided to describe
output files, which have equivalent names for each year. The
exception is files related to visibility analysis, which are
available only for 1992.

Note that Calpuff hourly output files (.DAT) are in binary format.
The NDDH used Lahey Fortran 95 to compile Calpuff, so the output
files will probably only be readable in programs compiled with
Lahey Fortran 90 or 95. (The provided SRCIN and Calpost
executables will work with those files).

The NDDH master source concentration files (containing source
contributions) are included in sub-directory SRCFILE of directory
OUTPUT. Due to space limitations, files are included only for
1990, 1991, and 1992. Again, these files are binary and will
probably only be readable in programs compiled with Lahey Fortran
90 or 95. (Lahey 95 compiled SRCOUT is provided). The Quattro Pro
spreadsheet used for evaluating visibility impact is included in
sub-directory QPRO.

Note that sub-sub-directory CONTROL of sub-directory PUFF of
directory INPUT includes a file named ALLSRC.DAT. This file
constitutes a composite inventory of all major and increment-
expanding sources modeled for the Class I increment analysis, in
Calpuff control file format (equivalent to Report Table 4-1).
While this composite inventory was not used in NDDH modeling, it
may be useful for verification modeling conducted by the reviewer.

Computer programs developed or modified by NDDH are included in
directory PROG. Index files are provided in the program sub-sub-
directories of sub-directory CODE. Programs related to geophysical

data preparation are included in sub-sub-directory PREGEO, and programs related to meteorological data preparation are in sub-sub-directory PREMET. CALPUFF5 (Calpuff Ver. 5.0, Lvl 971107) and CALPOST5 (Calpost Ver. 5.0, Lvl 971015) contain the versions used for the MRY Class I increment analysis. CALPUFF6 (Calpuff Ver. 5.0, Lvl 981116) and CALPOST6 (Calpost Ver. 5.0, Lvl 981116) contain the versions used for the MRY visibility analysis. The same version of Calmet (Calmet Ver. 5.0, Lvl 970825) was used for both analyses, and is included in sub-sub-directory CALMET5.